The Coupled Cluster Method and Entanglement

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Abstract: The Coupled Cluster (CC) and full CI expansions are studied for three fermions with six and seven modes. Surprisingly the CC expansion is tailor made to characterize the usual SLOCC entanglement classes. It means that the notion of a SLOCC transformation shows up quite naturally as a one relating the CC and CI expansions, and going from the CI expansion to the CC one is equivalent to obtaining a form for the state where the structure of the entanglement classes is transparent. In this picture entanglement is characterized by the parameters of the cluster operators describing transitions from occupied states to singles, doubles and triples of non occupied ones. Using the CC parametrization of states in the seven mode case we give a simple formula for the unique SLOCC invariant $\mathcal{J}$. Then we consider a perturbation problem featuring a state from the unique SLOCC class characterized by $\mathcal{J} \neq 0$. For this state with entanglement generated by doubles we investigate the phenomenon of changing the entanglement type due to the perturbing effect of triples. We show that there are states with real amplitudes such that their entanglement encoded into configurations of clusters of doubles is protected from errors generated by triples. Finally we put forward a proposal to use the parameters of the cluster operator describing transitions to doubles for entanglement characterization. Compared to the usual SLOCC classes this provides a coarse grained approach to fermionic entanglement.

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1 Introduction

According to the current paradigm quantum entanglement can be regarded as a new and efficient resource[1]. Suppose that we have a multipartite quantum system consisting of a number of subsystems. Entanglement can then be created between these subsystems via applying a set of *global* operations on the full system by switching on certain interactions. These can be effected via using successively a *discrete* sequence of quantum gates, or via applying a *continuous* evolution operator generated by some Hamiltonian. The particular type of entanglement obtained in this way is *defined* by prescribing a certain set of *local operations* acting on the *subsystems* that will result in *equivalent* states of the full system.

The most common operations used in quantum theory are of course the *unitary ones* resulting in unitary quantum gates and evolutions[1]. These are the ones leaving invariant the scalar products inherently connected to the structure of the multipartite space of states. Choosing the prescribed set as the *local* versions of such operations gives rise to the definition of entanglement classes as the set of equivalence classes of the space of states of the full system under the action of the group of *local unitary* (LU) transformations. Hence, two states are possessing the same entanglement if and only if they can be converted to each other via some local unitary transformation[2].

However, for practical purposes it turned out that this classification scheme is too restrictive[3, 4]. First of all, local unitary classification is providing a fine graining to the full set of states, whereas sometimes a coarse graining would be more desirable. Furthermore in quantum information processing manipulations of more general types then unitary ones are also allowed. These are physical manipulations (including communication between parties applying classical channels) resulting in the conversion of states back and forth with (generally different) success probabilities. These operations are called SLOCC operations (stochastic local operations and classical communication). They can be represented mathematically via the *local* action of the general linear group of *invertible* transformations of which the set of local unitary ones is merely a subgroup. The SLOCC entanglement classes are then defined as the equivalence classes of the set of states of the full system under the action of the group of local invertible SLOCC transformations. This new set of equivalence classes gives rise to a coarse graining of the space of states of the multipartite system.

Notice however, that unlike for a local unitary transformation the physical meaning for a particular local invertible one is not so obvious. Let us take the example of a multiqubit system. A local unitary transformation on a particular qubit is represented by a 2×2 unitary matrix which can be implemented by using physical equipment like Stern-Gerlach magnets, certain arrangements modelled by 2×2 Hamiltonians like the ones featuring the interaction of $1/2$ spins with external magnetic fields etc. On the other hand though being an elementary local invertible one the non unitary transformation $\begin{pmatrix} 1 & a \\ 0 & 1 \end{pmatrix}, a \in \mathbb{C}$ is not so easy to implement by a natural physical setup.

The notion of SLOCC classes can also be generalized to systems with indistinguishable constituents[5, 6]. Since the subsystems in this case are indistinguishable the local invertible transformations representing SLOCC manipulations should be identical. One can then ask what kind of physical representations of SLOCC transformations are available in this context? The aim of the present paper is to show that in the special case of choosing our system with indistinguishable constituents to be a fermionic one the notion of SLOCC transformations is intimately connected to a physically well established method used by quantum chemists for a long time. This method is the Coupled Cluster (CC) method[7, 8].

In the CC method the usual expansion of the state vector $|\Psi\rangle$ of the fermionic system given as a linear combination of Slater determinants (CI expansion) is replaced by a new one. The CC expansion is constructed via the action of a set of commuting cluster operators $e^{\hat{T}_i}$ $i = 1, 2, \dots$ on a special Slater determinant $|\Psi_0\rangle$ singled out by special physical considerations. The single particle states comprising $|\Psi_0\rangle$ are called the *occupied* ones. Then the cluster operators $\hat{T}_i$ describe single, double, triple etc. transitions from the occupied single particles states to non-occupied ones. Hence in this CC picture the state $|\Psi\rangle$ is regarded as a deviation from the distinguished state $|\Psi_0\rangle$ effected by multiple transitions from occupied states to non occupied ones.

In this paper by employing three-fermion systems with six[9, 10, 11] and seven[12] single particle states (modes) we would like to draw the readers attention to the fact that SLOCC transformations show up quite naturally within the framework of the CC method. In this context invertible transformations such as the aforementioned ones of upper triangular form are having a clear cut physical meaning. We also demonstrate that going from the CI expansion to the CC one plays the role of obtaining a form for a fermionic state where the structure of the SLOCC entanglement classes is transparent. The reason for restricting our attention merely to these special cases stems from the fact that apart from these ones (and the much more elaborate cases of three and four fermions with eight modes[13, 14]) the structure of the SLOCC classes and its invariants and covariants needed for our considerations is not known. Recall however, that precisely these special cases were the ones where the Borland-Dennis inequalities[15, 16] of quantum chemistry have been established. As is well-known by now these studies have given rise to recent developments culminating in the introduction of the generalized Pauli principle in connection with the famous N-representability problem[17, 18] and the idea of entanglement polytopes[19, 20]. In this spirit we conjecture that though illustrated merely in the simplest multipartite cases our results should have a generalization valid also for multi-fermionic systems with an arbitrary number of modes. We hope that

our observations will pave the way for interesting future applications.

The organization of this paper is as follows. In Section 2. we consider the case of three-fermionic systems with six modes. First by giving an explicit dictionary between the corresponding expansion coefficients we relate the CI and CC expansions. Then we look at the structure of the unique SLOCC invariant $\mathcal{D}$ of fourth order serving as a convenient measure of entanglement. We observe that there is a dramatic simplification in the structure of this invariant in the CC picture. In this case no contribution from the cluster operators $\hat{T}_1$ appears. It turns out that the reason for this is the fact that $\hat{T}_1$ generates SLOCC transformations, hence the corresponding term $e^{\hat{T}_1}$ can be removed from the expansion of $|\Psi\rangle$. Next we show that the remaining expansion coefficients related to $\hat{T}_2$ and $\hat{T}_3$ are characterizing the four nontrivial SLOCC entanglement classes in a simple manner. Section 3. is devoted to a study of the seven mode generalization of the results of Section 2. After recalling the structure of the basic invariant $\mathcal{J}$ of seventh order, the covariants and the SLOCC classes we again relate the CC and CI expansions. In the CC picture we find a surprisingly simple expression for $\mathcal{J}$. As a demonstration how the entanglement in this case is manifested in the structure of the cluster operators $\hat{T}_2$ and $\hat{T}_3$ we consider a perturbation problem. As a first step we choose a maximally entangled state defined by the condition $\mathcal{J} \neq 0$ which is generated merely by the expansion coefficients of $\hat{T}_2$ (doubles). Then we modify this state by adding also the contributions coming from $\hat{T}_3$ (triples). This perturbation due to triples is characterized by four complex numbers. As a next step we derive a constraint for the triples to be able to induce a transition to a different SLOCC class. It turns out that the constrained set of parameters define a six dimensional complex manifold which is known as the deformed conifold, i.e. a deformation of a six dimensional cone. Taking the perturbation parameters to be real reveals a new effect. If we change the sign of certain parameters of the doubles then the perturbation due to triples cannot induce a transition to a different SLOCC class. Hence in this special case the maximal entanglement encoded into the parameters of the doubles is protected from the perturbating effect of the triples. In section 4. we put forward a proposal to use the parameters of the cluster operators describing transitions to doubles for entanglement characterization. Compared to the usual SLOCC classes this provides a coarse grained approach to fermionic entanglement. Using our model systems familiar from Sections 2. and 3. and the new system of 4 fermions with 8 modes we offer some mathematical evidence supporting our proposal. Our conclusions and some comments are left to Section 5. For the convenience of the reader we put some of the technical details to an Appendix.

2 Three fermions with six modes

2.1 Relating the CI and CC expansions

We consider three fermions with six single particle states or modes. Let V be a six dimensional complex vector space and V^* its dual. We regard $V \simeq \mathbb{C}^6$ with $\{e_\mu\}, \mu = 1, 2, \ldots 6$ the canonical basis and $\{e^\mu\}$ is the dual basis. Elements of V will be called *single particle states* or modes. We tacitly assume that V is a Hilbert space also equipped with a Hermitian inner product, but we will not make use of this extra structure. We also introduce the twelve dimensional vector space

$$\mathcal{V} \equiv V \oplus V^*. \tag{1}$$

An element of $\mathcal{V}$ is of the form $x = v + \alpha$ where v is a vector and α is a linear form. In the case of fermions according to the method of second quantization to any element $x \in \mathcal{V}$ one can associate a linear operator $\hat{x}$ acting on the fermionic Fock space $\mathcal{F}$ as follows. We define fermionic creation and annihilation operators as

$$\hat{e}^\mu \equiv \hat{p}^\mu, \qquad \hat{e}_\mu \equiv \hat{n}_\mu, \qquad \mu = 1, \ldots 6 \tag{2}$$

satisfying the usual fermionic anticommutation relations

$$\{\hat{p}^\mu, \hat{n}_\nu\} = \delta^\mu_\nu \hat{1}, \qquad \{\hat{p}^\mu, \hat{p}^\nu\} = \{\hat{n}_\mu, \hat{n}_\nu\} = 0. \tag{3}$$

We define the vacuum state $|0\rangle \in \mathcal{F}$ by the property

$$\hat{n}_\mu|0\rangle = 0. \tag{4}$$

Then $\mathcal{F}$ is spanned by the basis vectors

$$\hat{p}^{\mu_1}\hat{p}^{\mu_2}\cdots\hat{p}^{\mu_k}|0\rangle, \qquad 1 \leq \mu_1 < \mu_2 < \cdots < \mu_k \leq 6. \tag{5}$$

In particular for $k = 3$ an unnormalized three fermion state with six modes can be written in the form

$$|\psi\rangle = \frac{1}{3!}\psi_{\mu\nu\rho}\hat{p}^\mu\hat{p}^\nu\hat{p}^\rho|0\rangle \tag{6}$$

where $\psi_{\mu\nu\rho}$ is totally antisymmetric having 20 independent complex amplitudes.

The SLOCC group is the one of invertible 6×6 matrices with complex entries i.e. $GL(6, \mathbb{C})$. It is acting on a state via transforming its amplitudes as

$$\psi_{\mu\nu\rho} \mapsto S_\mu{}^{\mu'}S_\nu{}^{\nu'}S_\rho{}^{\rho'}\psi_{\mu'\nu'\rho'}, \qquad S \in GL(6, \mathbb{C}). \tag{7}$$

Let us now split the single particle states to ones that are occupied and not occupied. The ones that are occupied will be labelled as

$$i, j, k = 1, 2, 3 \tag{8}$$

and the ones that are not as

$$a, b, c = \overline{1}, \overline{2}, \overline{3}. \tag{9}$$

Hence we have a new labelling for the six modes as

$$\{1, 2, 3, 4, 5, 6\} \equiv \{1, 2, 3, \overline{1}, \overline{2}, \overline{3}\}. \tag{10}$$

We take the Hartee-Fock (HF) state as the Slater determinant

$$|\psi_0\rangle \equiv \hat{p}^1\hat{p}^2\hat{p}^3|0\rangle. \tag{11}$$

We see that this distinguished element of $\mathcal{F}$ is built up from single particle states that are occupied. Now the Coupled Cluster (CC) and full CI expansions are respectively

$$|\psi\rangle = e^{\hat{T}_1+\hat{T}_2+\hat{T}_3}|\psi_0\rangle \tag{12}$$

and

$$|\psi\rangle = (\hat{1} + \hat{C}_1 + \hat{C}_2 + \hat{C}_3)|\psi_0\rangle. \tag{13}$$

Here

$$\hat{T}_1 = T_a{}^i\hat{p}^a\hat{n}_i, \qquad \hat{T}_2 = \frac{1}{4}T_{ab}{}^{ij}\hat{p}^a\hat{n}_i\hat{p}^b\hat{n}_j \qquad \hat{T}_3 = T_{\overline{123}}{}^{123}\hat{p}^{\overline{1}}\hat{n}_1\hat{p}^{\overline{2}}\hat{n}_2\hat{p}^{\overline{3}}\hat{n}_3 \tag{14}$$

and

$$\hat{C}_1 = C_a{}^i\hat{p}^a\hat{n}_i, \qquad \hat{C}_2 = \frac{1}{4}C_{ab}{}^{ij}\hat{p}^a\hat{n}_i\hat{p}^b\hat{n}_j \qquad \hat{C}_3 = C_{\overline{123}}{}^{123}\hat{p}^{\overline{1}}\hat{n}_1\hat{p}^{\overline{2}}\hat{n}_2\hat{p}^{\overline{3}}\hat{n}_3 \tag{15}$$

are called the cluster operators. Notice that by construction the set of operators $\{\hat{T}_1, \hat{T}_2, \hat{T}_3\}$ called *singles*, *doubles* and *triples* are commuting.

For the expansion coefficients of the "T"s and "C"s it will be useful to adopt the following labelling convention. First we relate the expansion of Eq.(6) in terms of the 20 komplex

numbers $\psi_{\mu\nu\varrho}$ and the 20 komplex numbers of the CI expansion in terms of the coefficients of the "C"s

$$1=\psi_{123}, \qquad {C_a}^i=\frac{1}{2}\varepsilon^{ijk}\psi_{jka}, \qquad {C_{ab}}^{ij}=\varepsilon^{ijk}\psi_{abk}, \qquad {C_{\overline{123}}}^{123}=\psi_{\overline{123}}. \tag{16}$$

For notational simplicity we rename the 20 numbers of this $1+9+9+1$ split in terms of two complex numbers α,β and two 3×3 matrices A,B as follows

$$\alpha=1, \qquad {A^a}_i=\frac{1}{4}\varepsilon^{abc}\varepsilon_{ijk}{C_{bc}}^{jk}, \qquad {B^i}_a={C_a}^i, \qquad \beta={C_{\overline{123}}}^{123}. \tag{17}$$

Similarly for the CCparameters we introduce yet another $1+9+9+1$ split featuring the complex numbers η,ξ and the 3×3 matrices X,Y

$$\eta=1, \qquad {X^a}_i=\frac{1}{4}\varepsilon^{abc}\varepsilon_{ijk}{T_{bc}}^{jk}, \qquad {Y^i}_a={T_a}^i, \qquad \xi={T_{\overline{123}}}^{123}. \tag{18}$$

In order to complete the dictionaries between the different expansions of Eq.(6),(12), and (13) we need to relate the sets (α,A,B,β) and (η,X,Y,ξ).

In order to do this let us also compare expansions (12) and (13). Then we get

$$\hat{C}_1=\hat{T}_1, \qquad \hat{C}_2=\hat{T}_2+\frac{1}{2}\hat{T}_1^2, \qquad \hat{C}_3=\hat{T}_3+\hat{T}_1\hat{T}_2+\frac{1}{6}\hat{T}_1^3 \tag{19}$$

$$\hat{T}_1=\hat{C}_1, \qquad \hat{T}_2=\hat{C}_2-\frac{1}{2}\hat{C}_1^2, \qquad \hat{T}_3=\hat{C}_3-\hat{C}_1\hat{C}_2+\frac{1}{3}\hat{C}_1^3. \tag{20}$$

One can check that

$$\hat{T}_1\hat{T}_2\hat{p}^1\hat{p}^2\hat{p}^3|0\rangle=\mathrm{Tr}(XY)\hat{p}^{\overline{1}}\hat{p}^{\overline{2}}\hat{p}^{\overline{3}}|0\rangle \tag{21}$$

$$\frac{1}{6}\hat{T}_1^3\hat{p}^1\hat{p}^2\hat{p}^3|0\rangle=(\mathrm{Det}Y)\hat{p}^{\overline{1}}\hat{p}^{\overline{2}}\hat{p}^{\overline{3}}|0\rangle \tag{22}$$

$$\frac{1}{2}\hat{T}_1^2\hat{p}^1\hat{p}^2\hat{p}^3|0\rangle={(Y^\sharp)^a}_i\varepsilon_{abc}\hat{p}^{\overline{i}}\hat{p}^b\hat{p}^c|0\rangle \tag{23}$$

$$\hat{T}_3\hat{p}^1\hat{p}^2\hat{p}^3|0\rangle=\xi\hat{p}^{\overline{1}}\hat{p}^{\overline{2}}\hat{p}^{\overline{3}}|0\rangle, \tag{24}$$

where $Y^\sharp$ is the adjoint matrix of Y i.e.

$$YY^\sharp=(\mathrm{Det}Y)I \tag{25}$$

with I the 3×3 identity matrix. Using these results by virtue of Eq.(19) we obtain the following dictionary between the CC and CI pictures

$$\alpha=\eta=1, \qquad B=Y, \qquad A=Y^\sharp+X, \qquad \beta=\mathrm{Det}Y+(X,Y)+\xi \tag{26}$$

where

$$(X,Y)\equiv\mathrm{Tr}(XY). \tag{27}$$

2.2 The quartic invariant

It is well-known that we have a quartic combination $\mathcal{D}(\psi)$ of the 20 amplitudes of $|\psi\rangle$ which is invariant under determinant one SLOCC transformations[9], i.e. under the action of the group $SL(6,\mathbb{C})$ of the form

$$\psi_{\mu\nu\rho}\mapsto {S_\mu}^{\mu'}{S_\nu}^{\nu'}{S_\rho}^{\rho'}\psi_{\mu'\nu'\rho'}, \qquad S\in SL(6,\mathbb{C}). \tag{28}$$

This invariant gives rise to a natural measure of fermionic entanglement which for embedded three-qubit states boils down[9] to the three-tangle describing the phenomenon of entanglement monogamy[21]. In order to introduce this invariant first we define the covariant[22, 12]

$$K^{\mu}{}_{\nu} = \frac{1}{12}\varepsilon^{\mu\rho_1\rho_2\rho_3\rho_4\rho_5}\psi_{\nu\rho_1\rho_2}\psi_{\rho_3\rho_4\rho_5} \tag{29}$$

which is transforming under SLOCC as

$$K^{\mu}{}_{\nu} \mapsto (\mathrm{Det}S)S^{\mu}{}_{\mu'}S'_{\nu}{}^{\nu'}K^{\mu'}{}_{\nu'} \tag{30}$$

where $S' = S^{-1T}$. Then

$$\mathcal{D}(\psi) = \frac{1}{6}\mathrm{Tr}(K^2) = \frac{1}{6}K^{\mu}{}_{\nu}K^{\nu}{}_{\mu}. \tag{31}$$

Hence it follows that $\mathcal{D}(\psi)$ is a relative invariant under SLOCC i.e.

$$\mathcal{D}(\psi) \mapsto (\mathrm{DetS})^2\mathcal{D}(\psi) \tag{32}$$

and invariant under the $SL(6,\mathbb{C})$ SLOCC subgroup.

We will need the expression for $\mathcal{D}(\psi)$ in the parametrization of Eq.(17). It is given by the formula[9]

$$\mathcal{D}(\psi) = 4[\kappa^2 - (A^\sharp, B^\sharp) + \alpha\mathrm{Det}A + \beta\mathrm{Det}B], \qquad 2\kappa = \alpha\beta - (A, B). \tag{33}$$

This expression displays the parameters (α, A, B, β) i.e. the ones of the full CI expansion of $|\psi\rangle$ of (13). Using Eq. (26) let us now give its new expression in terms of the CC expansion parameters (η, Y, X, ξ). The result is the much simpler expression

$$\mathcal{D}(\psi) = \xi^2 + 4\mathrm{Det}X. \tag{34}$$

Hence this expression is not featuring the matrix Y at all!

Looking back at Eq.(33) we see that the alternative choice

$$\alpha' = 1, \qquad B' = 0, \qquad A' = X, \qquad \beta' = \xi \tag{35}$$

obtained by setting $Y = 0$ in Eq.(26) immediately yields Eq.(34). Hence we suspect that the states $|\psi\rangle$ answering the set (α, A, B, β) and $|\psi'\rangle$ answering the one $(\alpha', A', B', \beta')$ are related by a special $SL(6,\mathbb{C})$ transformation.

This is indeed the case. The group $SL(6,\mathbb{C})$ is having a subgroup of upper triangular matrices of the form

$$\begin{pmatrix} I & \Lambda \\ 0 & I \end{pmatrix}, \qquad \Lambda \in Matr(3,\mathbb{C}). \tag{36}$$

In the language of the set (α, A, B, β) these transformations are of the form[9]

$$\alpha' = \alpha, \qquad B' = B + \alpha\Lambda, \qquad A' = A + 2B\times\Lambda + \alpha\Lambda^\sharp \tag{37}$$

$$\beta' = \beta + (A,\Lambda) + (B,\Lambda^\sharp) + \alpha\mathrm{Det}\Lambda \tag{38}$$

where

$$2B\times\Lambda = (B+\Lambda)^\sharp - B^\sharp - \Lambda^\sharp. \tag{39}$$

Now we can see that with the choice

$$\Lambda \equiv -Y \tag{40}$$

from the set of Eq.(26) we can obtain the one of Eq.(35). The upshot of these considerations is that using a SLOCC transformation corresponding to the matrix of Eq.(36) with parameter

given by (40) we can get rid of the $\hat{T}_1$ term in the CC expansion of Eq.(12). Hence in order to reveal the interplay between the CCM and the SLOCC classes it is sufficient to examine the structure of the state

$$|\psi'\rangle = e^{\hat{T}_2+\hat{T}_3}|\psi_0\rangle \tag{41}$$

with parameters given by (35).

It is easy to see that this important conclusion is valid also in the most general case (i.e. the number of modes can be arbitrary, say N). Indeed, since the operators $\hat{T}_1, \hat{T}_2$ and $\hat{T}_3$ are commuting ones we can write

$$|\psi\rangle = e^{\hat{T}_1}e^{\hat{T}_2}e^{\hat{T}_3}|\psi_0\rangle. \tag{42}$$

Now it is easy to check that the operator $e^{\hat{T}_1}$ always generates SLOCC transformations of upper triangular form. To cap all this our observation is valid for an arbitrary number of (say n) fermions so one can write

$$|\Psi\rangle = e^{\hat{T}_1}|\Psi'\rangle, \qquad |\Psi'\rangle = e^{\hat{T}_2}\cdots e^{\hat{T}_n}|\Psi_0\rangle, \qquad e^{\hat{T}_1} \in GL(N,\mathbb{C}) \tag{43}$$

where

$$|\Psi_0\rangle \equiv \hat{p}^1\hat{p}^2\cdots\hat{p}^n|0\rangle. \tag{44}$$

Hence again $|\Psi\rangle$ and $|\Psi'\rangle$ are in the same SLOCC class. In summary: in the CC picture SLOCC entanglement is characterized merely by the cluster operators $\hat{T}_2, \dots, \hat{T}_n$. Then the CC expansion featuring only these operators represent deviations from the separable class represented by a single Slater determinant i.e. a HF state of the form

$$|\Psi_B\rangle \equiv e^{\hat{T}_1}|\Psi_0\rangle. \tag{45}$$

The state $|\Psi_B\rangle$ can also be written as a single Slater determinant in a suitable basis. In the case of our example of three fermions with six modes we have

$$|\psi_B\rangle = e^{\hat{T}_1}|\psi_0\rangle = (\hat{p}^1 + Y^1{}_a\hat{p}^a)(\hat{p}^2 + Y^2{}_b\hat{p}^b)(\hat{p}^3 + Y^3{}_c\hat{p}^c)|0\rangle. \tag{46}$$

2.3 SLOCC classes and CCM

As described elsewhere[9] given a state $|\psi\rangle$ one can introduce a dual state $|\tilde{\psi}\rangle$ which is a cubic expression of the original amplitudes of $|\psi\rangle$ as follows

$$|\tilde{\psi}\rangle \longleftrightarrow (\tilde{\alpha}, \tilde{A}, \tilde{B}, \tilde{\beta}) \tag{47}$$

$$\tilde{\alpha} = 2\alpha\kappa + 2\mathrm{Det}B, \qquad \tilde{A} = 2(\beta B^\sharp - 2B \times A^\sharp) - 2\kappa A. \tag{48}$$

$$\tilde{\beta} = -2\beta\kappa - 2\mathrm{Det}A, \qquad \tilde{B} = -2(\alpha A^\sharp - 2A \times B^\sharp) + 2\kappa B, \tag{49}$$

where κ and the cross product are defined in Eqs.(33) and (39). One can also introduce the following set of quadratic polynomials

$$Q_1 = \alpha\beta I - AB, \qquad Q_2 \equiv A^\sharp - \beta B, \qquad Q_3 \equiv B^\sharp - \alpha A. \tag{50}$$

In fact these 3×3 matrices are just coming from the blocks of the covariant of Eq.(29) hence $K_\psi = 0$ iff $Q_1 = Q_2 = Q_3 = 0$. Then it is known[9, 12] that the SLOCC classes can be characterized as follows.

Let us denote by $\mathcal{M}_0$ our space of three fermions with six modes. Clearly $\mathcal{M}_0 \simeq \wedge^3\mathbb{C}^6$. We make the further definitions

$$\mathcal{M}_1 \equiv \{\psi \in \mathcal{M}_0 | \mathcal{D}(\psi) = 0\} \tag{51}$$

$$\mathcal{M}_2 \equiv \{\psi \in \mathcal{M}_0 | \mathcal{D}(\psi) = 0, \tilde{\psi} = 0\} \tag{52}$$

$$\mathcal{M}_3 \equiv \{\psi \in \mathcal{M}_0 | K_\psi = 0\} \tag{53}$$

Notice that in the case of $\mathcal{M}_3$ the vanishing of the covariant K_ψ automatically implies $\mathcal{D}(\psi) = 0, \tilde{\psi} = 0$. Now we have[9] four nontrivial $GL(6, \mathbb{C})$ orbits which we call SLOCC entanglement classes

$$\mathcal{O}_{GHZ} \equiv \mathcal{M}_0 - \mathcal{M}_1 = [(\hat{p}^{123} + \hat{p}^{1\overline{23}} + \hat{p}^{\overline{1}2\overline{3}} + \hat{p}^{\overline{12}3}|0\rangle)] \tag{54}$$

$$\mathcal{O}_W \equiv \mathcal{M}_1 - \mathcal{M}_2 = [(\hat{p}^{123} + \hat{p}^{1\overline{23}} + \hat{p}^{\overline{1}2\overline{3}}|0\rangle)] \tag{55}$$

$$\mathcal{O}_{BISEP} \equiv \mathcal{M}_2 - \mathcal{M}_3 = [(\hat{p}^{123} + \hat{p}^{1\overline{23}}|0\rangle)] \tag{56}$$

$$\mathcal{O}_{SEP} \equiv \mathcal{M}_3 = [\hat{p}^{123}|0\rangle] \tag{57}$$

where the notation $[|\psi\rangle]$ refers to the SLOCC orbit (equivalence class) of the unnormalized state $|\psi\rangle$

The SEP (separable) class is the class consisting of states that can be written as a single Slater determinant. The BISEP (biseparable) class corresponds to the set of tripartite states that can be transformed via SLOCC to states consisting of the sum of two Slater determinants containing a common factor of single particle states. The W and GHZ classes form the genuine entanglement classes. The names separable, biseparable, W and GHZ are originating from the fact that when considering embedded three-qubit systems living inside our three fermionic ones[9, 10] these classes correspond to the separable, biseparable, W and GHZ classes known from studies of three-qubit entanglement[4].

Since $\mathcal{D}$ is a $SL(6, \mathbb{C})$ invariant and $|\tilde{\psi}\rangle$ and K are covariants one can calculate these quantities merely for the transformed representative $|\psi'\rangle$ also belonging to the orbit of $|\psi\rangle$. Using Eq.(35) one obtains

$$\tilde{\alpha}' = \xi, \qquad \tilde{A}' = -\xi X, \qquad \tilde{B}' = -2X^\sharp, \qquad \tilde{\beta}' = -\xi^2 - 2\mathrm{Det}X \tag{58}$$

$$Q'_1 = \xi I, \qquad Q'_2 = X^\sharp, \qquad Q'_3 = -X. \tag{59}$$

From these results we see that:

I. The matrix Y plays no role in the SLOCC classes.

II. The SEP (single Slater determinant) states are **precisely** the states characterized by the constraints $\xi = 0$ and $X = 0$. For these states $\mathcal{D}$, $|\tilde{\Psi}\rangle$ and K_ψ are vanishing automatically.

III. The BISEP states are characterized by the constraints $\xi = 0$, $X^\sharp = 0$, DetX=0 but $X \neq 0$. These constraints automatically yield $\mathcal{D} = 0$ and $|\tilde{\Psi}\rangle = 0$, however $K_\psi \neq 0$.

IV. The W states are characterized by the constraint $\xi^2 + 4\mathrm{Det}X = 0$, and the nonvanishing of *at least one* of the quantities of Eq.(58). So for instance we are in the W-class if we have $\xi = 0, X \neq 0, X^\sharp \neq 0, \mathrm{Det}X = 0$.

V. The GHZ states are characterized by the constraint $\xi^2 + 4\mathrm{Det}X \neq 0$. These states are *dense* within the full set of states.

Recall that ξ and X characterize the contributions coming from triples and doubles of cluster operators. From the above results we also see that in order to find out which entanglement class a state belongs the derived quantities of $X^\sharp$ and $\mathrm{Det}X$ should also to be taken into consideration. Summarizing: interestingly the notion of a SLOCC transformation shows up quite naturally as a one relating the CC and CI expansions. Going from the CI expansion to the CC one seems to play the role of obtaining something like a simplified form for the three fermion state where the structure of the entanglement classes is transparent. In order to see how our observations generalize in the next section we turn to a more complicated system.

3 Three fermions with seven single particle states

3.1 Invariants and covariants

A three fermion state with seven modes can be written in the following form

$$|\Psi\rangle = \frac{1}{3!}\Psi_{IJK}\hat{p}^{IJK}|0\rangle \tag{60}$$

where $I, J, K = 1, 2, \ldots 7$ and Ψ_{IJK} is a totally antisymmetric complex tensor having 35 independent components. The SLOCC group is $GL(7, \mathbb{C})$ and the group action is the usual one

$$\Psi_{IJK} \mapsto S_I{}^{I'} S_J{}^{J'} S_K{}^{K'} \Psi_{I'J'K'}, \qquad S \in GL(7, \mathbb{C}). \tag{61}$$

The basic covariants are[12]

$$(M^I)^J{}_K = \frac{1}{12}\varepsilon^{IJA_1A_2A_3A_4A_5}\Psi_{KA_1A_2}\Psi_{A_3A_4A_5} \tag{62}$$

$$N_{IJ} = \frac{1}{24}\varepsilon^{A_1A_2A_3A_4A_5A_6A_7}\Psi_{IA_1A_2}\Psi_{JA_3A_4}\Psi_{A_5A_6A_7} \tag{63}$$

$$L^{IJ} = (M^I)^{A_1}{}_{A_2}(M^J)^{A_2}{}_{A_1}. \tag{64}$$

Under SLOCC the transformation properties of these covariants are as follows

$$(M^I)^J{}_K \mapsto (\mathrm{Det}S) S^I{}_{I'} S^J{}_{J'} S'_K{}^{K'} (M^{I'})^{J'}{}_{K'} \tag{65}$$

$$N_{IJ} \mapsto (\mathrm{Det}S) S'_I{}^{I'} S'_J{}^{J'} N_{I'J'} \tag{66}$$

$$L^{IJ} \mapsto (\mathrm{Det}S)^2 S^I{}_{I'} S^J{}_{J'} L^{I'J'} \tag{67}$$

where $S' = (S^{-1})^T$. Notice that the 7×7 matrices N_{IJ} and L^{IJ} are symmetric.

From these covariants one can form a unique algebraically independent relative invariant

$$\mathcal{J}(\Psi) = \frac{1}{2^4 \cdot 3^2 \cdot 7}\mathrm{Tr}(NL) = \frac{1}{2^4 \cdot 3^2 \cdot 7} N_{IJ} L^{IJ}. \tag{68}$$

$\mathcal{J}$ is a relative invariant meaning that under SLOCC it picks up a determinant factor

$$\mathcal{J}(\Psi) \mapsto (\mathrm{Det}S)^3 \mathcal{J}(\Psi) \tag{69}$$

hence it is invariant under the SLOCC subgroup $SL(7, \mathbb{C})$. Defining

$$\mathcal{B}_{IJ} = -\frac{1}{6}N_{IJ} \tag{70}$$

we have the alternative formula

$$(\mathcal{J}(\Psi))^3 = \mathrm{Det}\mathcal{B}. \tag{71}$$

3.2 Relating the CC and CI expansions for seven modes

Similarly to the six mode case for a coupled cluster description of this three fermion system we split the modes to ones that are occupied labelled by $i, j, k = 1, 2, 3$ and the ones that are not occupied by $a, b, c = \overline{1}, \overline{2}, \overline{3}, \overline{4}$. Now the CC and CI expansions will be just the same form as the ones displayed in Eqs.(11)-(15) with the exception of $\hat{T}_3$ and $\hat{C}_3$ having the new form

$$\hat{T}_3 = \frac{1}{3!}T_{abc}{}^{123}\hat{p}^a\hat{n}_1\hat{p}^b\hat{n}_2\hat{p}^c\hat{n}_3, \qquad \hat{C}_3 = \frac{1}{3!}C_{abc}{}^{123}\hat{p}^a\hat{n}_1\hat{p}^b\hat{n}_2\hat{p}^c\hat{n}_3. \tag{72}$$

It is rewarding to tackle this case as a deviation from the six mode one. We write

$$|\Psi\rangle = |\psi\rangle + |\omega\rangle, \qquad |\omega\rangle = \frac{1}{2}\omega_{\mu\nu}\hat{p}^{\mu\nu\overline{4}}|0\rangle \tag{73}$$

and $|\psi\rangle$ is given by Eq.(6). The 6×6 antisymmetric matrix ω has 15 independent components. We write

$$\omega \equiv \begin{pmatrix} E & D \\ -D^T & F \end{pmatrix} \tag{74}$$

where E, F are two 3×3 antisymmetric matrices and D is an arbitrary 3×3 matrix. Hence in the CI and CC pictures we group the 35 amplitudes to three 3×3 matrices, and two 3×3 antisymmetric ones so in the CI picture we will have five matrices A, B, D, E, F with the latter two being antisymmetric, and two scalars α and β. Similarly in the CC picture the five matrices will be denoted as X, Y, Z, U, V with the latter two antisymmetric, and the corresponding scalars are η and ξ. The scalars and the first two matrices in both pictures have already been defined by Eqs.(17) and (18). The remaining matrices are defined as

$$C_{a\overline{4}}{}^{ij} = \varepsilon^{ijk}\Psi_{ka\overline{4}} = \varepsilon^{ijk}D_{ka}, \qquad C_{\overline{4}}{}^{i} = \frac{1}{2}\varepsilon^{ijk}\Psi_{jk\overline{4}} = \frac{1}{2}\varepsilon^{ijk}E_{jk} \tag{75}$$

$$C_{ab\overline{4}}{}^{123} = \Psi_{ab\overline{4}} = F_{ab}. \tag{76}$$

$$T_{a\overline{4}}{}^{ij} = \varepsilon^{ijk}Z_{ka}, \qquad T_{\overline{4}}{}^{i} = \frac{1}{2}\varepsilon^{ijk}V_{jk}, \qquad T_{ab\overline{4}}{}^{123} = U_{ab} \tag{77}$$

where in these expressions we have $a, b = \overline{1}, \overline{2}, \overline{3}$.

Now similarly to the six mode case we expect that the form of the unique relative invariant $\mathcal{J}(\Psi)$ of Eq.(68) will be of much simpler form in the CC than in the CI picture. Indeed, in the next subsection it turns out that unlike in the CI picture where this invariant is featuring all of the amplitudes $(\alpha, \beta, A, B, D, E, F)$ in the CC one only the quantities $(\eta = 1, \xi, X, Z, U)$ show up.

In order to prove this again we have to relate the CI and CC amplitudes using Eq.(19). Then a calculation shows that

$$\alpha = \eta = 1, \qquad \beta = \xi + \mathrm{Tr}(XY) + \mathrm{Det}Y, \qquad B = Y, \qquad A = X + Y^{\sharp} \tag{78}$$

$$D = Z + VY, \qquad E = V, \qquad F = U + (Z^TY - Y^TZ) + [(X + Y^{\sharp})v]. \tag{79}$$

Here

$$v^i = \frac{1}{2}\varepsilon^{ijk}V_{jk}, \qquad V_{ij} \equiv [v]_{ij} = \varepsilon_{ijk}v^k \tag{80}$$

i.e. the latter notation refers to building up a 3×3 antisymmetric matrix from a 3 component vector.

3.3 The seventh order invariant

The data $(\alpha, \beta, A, B, D, E, F)$ described in the previous section is directly related to the complex amlitudes Ψ_{IJK}. They can be used for calculating the covariants and the invariant of Eq.(68). Again the data connected to the operator $\hat{T}_1$ is not needed since it can be linked to a SLOCC transformation of upper triangular form. It means that it is enough to do the calculation with $V = Y = 0$. The result for the calculation of the components of the covariants N_{IJ} and M^{IJ} is given in the Appendix. Putting everything together the final result is the surprisingly simple expression

$$\mathcal{J}(\Psi) = -\mathrm{Det}(G) - \frac{1}{4\xi}\mathrm{Det}(UX + \xi Z^T), \qquad G \equiv \frac{1}{2}(ZX + X^TZ^T), \tag{81}$$

where the matrix G is just the symmetric part of the 3×3 matrix ZX. Notice that the expression is regular for $\xi=0$ since for arbitrary 3×3 matrices we have

$$\mathrm{Det}(A+B)=\mathrm{Det}A+\mathrm{Tr}(A^{\sharp}B)+\mathrm{Tr}(AB^{\sharp})+\mathrm{Det}B, \tag{82}$$

and $\mathrm{Det}UX=0$ due to $U^T=-U$.

Let us find inside this formula our invariant of Eq.(34) familiar from the six mode case! First notice that due to Eq.(80) and the antisymmetry of U we have $uu^T=U^{\sharp}$. Then introducing yet another 3 component vector w and its corresponding antisymmetric matrix $W\equiv[w]$ as

$$W\equiv\frac{1}{2}(ZX-X^TZ^T),\qquad w^i=\frac{1}{4}\varepsilon^{ijk}(ZX-X^TZ^T)_{jk} \tag{83}$$

we obtain

$$\mathcal{J}(\Psi)=w^TGw-\frac{1}{4}u^THu-\frac{1}{4}\left(\mathrm{Det}Z(\xi^2+4\mathrm{Det}X)\right)-\frac{1}{4}\xi\mathrm{Tr}(UXZ^{T\sharp}), \tag{84}$$

$$H=\frac{1}{2}(Z^TX^{\sharp}+X^{\sharp T}Z). \tag{85}$$

Here we also used that

$$\mathrm{Det}(ZX)=\mathrm{Det}(W+G)=\mathrm{Det}G+Tr(W^{\sharp}G)=\mathrm{Det}G+w^TGw. \tag{86}$$

From Eq.(81) it is also clear that if we have $G=ZX$ (i.e. when the matrix ZX is symmetric) and $U=0$ then $\mathcal{J}(\Psi)=-\mathrm{Det}Z(\xi^2+4\mathrm{Det}X)/4$.

An equivalent way of formulating this can be given as follows. Define $\hat{\omega}=\frac{1}{2}\omega_{\mu\nu}\hat{p}^{\mu\nu\overline{4}}$ and apply the restricion $Y=V=0$. Then according to Eq.(79) then $D=Z$, $E=0$ and $F=U$ hence one can verify that

$$\hat{\omega}|\psi\rangle=0\qquad\text{iff}\qquad G=ZX,\quad U=0. \tag{87}$$

Recall that $\mathrm{Det}\omega=(\mathrm{Pf}\omega)^2$ where

$$\mathrm{Pf}(\omega)=\frac{1}{2^3 3!}\varepsilon^{\mu_1\mu_2\mu_3\mu_4\mu_5\mu_6}\omega_{\mu_1\mu_2}\omega_{\mu_3\mu_4}\omega_{\mu_5\mu_6} \tag{88}$$

then in the case when $V=U=Y=0$ we have $\mathrm{DetZ}=-\mathrm{Pf}\omega$. Using this one obtains the result

$$\mathcal{J}(\Psi)=\frac{1}{4}\mathrm{Pf}(\omega)\mathcal{D}(\psi). \tag{89}$$

It can be proved that this result remains valid also in the case when the restrictions $V=Y=0$ are removed[12]. Hence $\hat{\omega}|\psi\rangle=0$ of Eq.(87) can be regarded as a necessary condition for the separability of the seventh order invariant to a cubic and a quartic one.

3.4 Entanglement classes

The SLOCC classification of three-fermion states with seven modes is known in the mathematical literature as the classification problem of three-forms in a seven dimesional vector space[23, 24, 25]. These results has recently been introduced to entanglement theory[12]. Here we would like to recall the structure of the SLOCC classes.

Let us consider the state

$$|\Psi_-\rangle=(\hat{p}^{123}-\hat{p}^{1\overline{23}}-\hat{p}^{2\overline{31}}-\hat{p}^{3\overline{12}}+\hat{p}^{1\overline{14}}+\hat{p}^{2\overline{24}}+\hat{p}^{3\overline{34}})|0\rangle. \tag{90}$$

In this special case due to relations (78)-(79) we have

$$(\alpha,A,B,\beta,D,E,F)=(\eta,X,Y,\xi,Z,V,U)=(1,-I,0,0,I,0,0). \tag{91}$$

(Notice that according to our findings at the end of Section 2.2. one can always achieve that $V = Y = 0$ and in this case by virtue of Eqs.(78) and (79) the CC and CI labels are just the same.) Using now Eq.(81) with $Z = -X = I$, and $\xi = U = 0$ we obtain

$$\mathcal{J}(\Psi_-) = 1. \tag{92}$$

It can be shown[12] that this three-fermion state with seven modes belongs to a dense SLOCC orbit characterized by the property $\mathcal{J}(\Psi_-) \neq 0$. Notice that from the mathematical point of view this orbit is similar to the dense SLOCC orbit of the famous GHZ state of the six mode case for which we had $\mathcal{D} \neq 0$. Indeed apart from some signs the first four terms of Eq.(90) correspond to a structure already known from Eq.(54).

In order to make the connection with the three-qubit GHZ-state more explicit we introduce the complex linear combinations

$$\hat{E}^{1,2,3} = \hat{p}^{1,2,3} + i\hat{p}^{\overline{1},\overline{2},\overline{3}}, \qquad \hat{E}^{\overline{1},\overline{2},\overline{3}} = \hat{p}^{1,2,3} - i\hat{p}^{\overline{1},\overline{2},\overline{3}}, \qquad \hat{E}^{\overline{4}} = i\hat{p}^{\overline{4}}. \tag{93}$$

Then one can write

$$\left(\hat{p}^{123} - \hat{p}^{1\overline{23}} - \hat{p}^{\overline{1}2\overline{3}} - \hat{p}^{\overline{12}3}\right)|0\rangle = \frac{1}{2}\left(\hat{E}^{123} + \hat{E}^{\overline{123}}\right)|0\rangle. \tag{94}$$

Then the state on the right hand side of Eq.(94) corresponds to the structure $|000\rangle + |111\rangle$ of the unnormalized three-qubit GHZ state. It can be proved that the correpondence is not superficial since the three-qubit SLOCC group can be embedded in a consistent manner to the fermionic SLOCC one[9, 10]. Now our state of Eq.(90) can be given the following form

$$|\Psi_-\rangle = \frac{1}{2}\left(\hat{E}^{123} + \hat{E}^{\overline{123}} + (\hat{E}^{1\overline{1}} + \hat{E}^{2\overline{2}} + \hat{E}^{3\overline{3}})\hat{E}^{\overline{4}}\right)|0\rangle. \tag{95}$$

The reason for the notation $|\Psi_-\rangle$ corresponds to the fact that according to the left hand side of Eq.(94) and Eq.(34) the $\mathcal{D}$ invariant of the GHZ-part is negative (see also Eq.(89) and the preceeding discussion).

Now introducing the notation

$$|\Psi\rangle \equiv \hat{\Psi}|0\rangle \tag{96}$$

the SLOCC entanglement classes are given in Table 1. We note that for a full characterization of these classes other covariants are also needed[12]. However, for our purposes it is sufficient to consider merely the quantities N_{IJ} and $\mathcal{J}$. Notice also that according to Eq.(74) the 6×6 antisymmetric matrix defines an alternating (symplectic) form on the six dimensional space of single particle states. Then the operator $\hat{E}^{1\overline{1}} + \hat{E}^{2\overline{2}} + \hat{E}^{3\overline{3}}$ defines a canonical form for a nondegenerate symplectic form. This explains the abbreviation SYMPL showing up in the second column of our table. The other abbreviations conform with our ones familiar from Eqs.(54)-(57).

3.5 Perturbing the canonical GHZ-like state

In this section we would like to obtain an insight into the interplay between the structure of cluster operators $\hat{T}_2$ and $\hat{T}_3$ and the entanglement classes of the previous section. In order to achieve this as a first step notice that in our description of the SLOCC classes for three-fermions with seven modes we managed to produce the "GHZ-like" state $|\Psi_-\rangle$ belonging to the dense orbit merely via an application of cluster operators containing only doubles. This means that when building up this state only the expansion coefficients of $\hat{T}_2$ were used (see Eqs.(18), (77) and (91)).

Now we would like to perturb this state by adding to it a new term which is also containing contribution from triples i.e. from the expansion coefficients of the operator $\hat{T}_3$. To this end we choose

$$|\Phi_-\rangle = |\Psi_-\rangle + |\chi\rangle, \qquad |\chi\rangle = \left(\xi\hat{p}^{\overline{123}} + u^{\overline{1}}\hat{p}^{\overline{234}} + u^{\overline{2}}\hat{p}^{\overline{314}} + u^{\overline{3}}\hat{p}^{\overline{124}}\right)|0\rangle. \tag{97}$$

Name	Type	Canonical form of $\hat{\Psi}$	Rank $N_{IJ}(\Psi)$	$\mathcal{J}(\Psi)$
I	NULL	0	0	0
II	SEP	$\hat{E}^{123}$	0	0
III	BISEP	$\hat{E}^{1}(\hat{E}^{23}+\hat{E}^{\bar{2}\bar{3}})$	0	0
IV	W	$\hat{E}^{12\bar{3}}+\hat{E}^{1\bar{2}3}+\hat{E}^{\bar{1}23}$	0	0
V	GHZ	$\hat{E}^{123}+\hat{E}^{\bar{1}\bar{2}\bar{3}}$	0	0
VI	SYMPL/NULL	$(\hat{E}^{1\bar{1}}+\hat{E}^{2\bar{2}}+\hat{E}^{3\bar{3}})\hat{E}^{\overline{4}}$	1	0
VII	SYMPL/SEP	$(\hat{E}^{1\bar{1}}+\hat{E}^{2\bar{2}}+\hat{E}^{3\bar{3}})\hat{E}^{\overline{4}}+\hat{E}^{123}$	1	0
VIII	SYMPL/BISEP	$(\hat{E}^{1\bar{1}}+\hat{E}^{2\bar{2}}+\hat{E}^{3\bar{3}})\hat{E}^{\overline{4}}+\hat{E}^{1}(\hat{E}^{23}+\hat{E}^{\bar{2}\bar{3}})$	2	0
IX	SYMPL/W	$(\hat{E}^{1\bar{1}}+\hat{E}^{2\bar{2}}+\hat{E}^{3\bar{3}})\hat{E}^{\overline{4}}+\hat{E}^{12\bar{3}}+\hat{E}^{1\bar{2}3}+\hat{E}^{\bar{1}23}$	4	0
X	SYMPL/GHZ	$(\hat{E}^{1\bar{1}}+\hat{E}^{2\bar{2}}+\hat{E}^{3\bar{3}})E^{\overline{4}}+\hat{E}^{123}+\hat{E}^{\bar{1}\bar{2}\bar{3}}$	7	$\neq 0$

Table 1: Entanglement classes of three fermions with seven single particle states. Representative states of the SLOCC classes are obtained by acting with $\hat{\Psi}$ on the vacuum as in Eq.(96). The covariant N_{IJ} and invariant $\mathcal{J}$ are defined by Eqs.(63) and (68).

Using Eq.(68) we obtain

$$\mathcal{J}(\Phi_-) = 1 - \frac{1}{4}\left(\xi^2 + (u^{\overline{1}})^2 + (u^{\overline{2}})^2 + (u^{\overline{3}})^2\right). \tag{98}$$

Hence we remain in the dense orbit unless the condition

$$\xi^2 + (u^{\overline{1}})^2 + (u^{\overline{2}})^2 + (u^{\overline{3}})^2 = 4. \tag{99}$$

holds. Notice that the equation

$$\xi^2 + (u^{\overline{1}})^2 + (u^{\overline{2}})^2 + (u^{\overline{3}})^2 = 0. \tag{100}$$

defines a six dimensional conifold[26]. Just as a two-dimensional cone is embedded in real three-dimensional space as $x^2 + y^2 - z^2 = 0$, a real six dimensional conifold is embedded in $\mathbb{C}^4$ via Eq.(100). The conifold is a smooth space apart from a singularity at $\xi = u^{\overline{1}} = u^{\overline{2}} = u^{\overline{3}} = 0$. It is known[26] that one way to repair this singularity is given by a process called deformation under which Eq.(100) is modified to

$$\xi^2 + (u^{\overline{1}})^2 + (u^{\overline{2}})^2 + (u^{\overline{3}})^2 = Q^2 \tag{101}$$

where Q is a real deformation parameter. Now we see that Eq.(99) giving the condition needed for leaving the dense SLOCC orbit is the one of the perturbing parameters coming from triples defining a deformed conifold with the special deformation parameter $Q = 2$.

For real parameters $(\xi, u^a) \in \mathbb{R}^4$ this means that if the 4 parameters corresponding to the cluster operators describing triples are belonging to a three dimensional sphere of radius 2 then the entanglement type is changed. The parametrized family of three fermion states in this case leaves the dense orbit. From Table. 1. we see that apart from the entanglement class corresponding to the dense SLOCC orbit, we have 9 more classes[1]. As a next step we show how this class can be identified.

In order to do this we calculate the covariant N_{IJ} a symmetric 7×7 matrix and look at how its rank is behaving as we reach the singular locus of $\mathcal{J}(\Phi_-)$. Rather than using the matrix N_{IJ} for convenience we use the one $\mathcal{B}_{IJ} = -\frac{1}{6}N_{IJ}$ of Eq.(70). For the state $|\Psi_-\rangle$ this new matrix becomes just the identity matrix, i.e. we have $\mathcal{B}_{IJ} = \delta_{IJ}$. Using the expressions given in the Appendix for the perturbed state we get

$$\mathcal{B}_{IJ}(\Phi_-) = \begin{pmatrix} I & -\frac{1}{2}(\xi I + U) & -\frac{1}{2}u \\ -\frac{1}{2}(\xi I - U) & I & 0 \\ -\frac{1}{2}u^T & 0 & 1 \end{pmatrix}. \tag{102}$$

[1] Taken together with the trivial class represented by the zero state.

By applying a suitable (generally complex) orthogonal matrix we can diagonalize $\mathcal{B}$

$$\mathcal{B}^{\text{diag}} = S^T \mathcal{B} S, \qquad S = \frac{1}{\sqrt{2}Q}\begin{pmatrix} QI & QI & 0 \\ \xi I - U & U - \xi I & \sqrt{2}u \\ u^T & -u^T & -\sqrt{2}\xi \end{pmatrix} \in SO(7, \mathbb{C}) \tag{103}$$

$$\mathcal{B}^{\text{diag}} = \begin{pmatrix} \left(1 - \frac{1}{2}Q\right) I & 0 & 0 \\ 0 & \left(1 + \frac{1}{2}Q\right) I & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{104}$$

where

$$Q \equiv \sqrt{\xi^2 + (u^{\overline{1}})^2 + (u^{\overline{2}})^2 + (u^{\overline{3}})^2} \tag{105}$$

and recall also our conventions of Eq.(80). From Eq.(71) we see that we are in accord with Eq.(98) and also see that our matrix $\mathcal{B}$ fails to be of full rank if the (99) i.e. $Q = 2$ condition holds. From Eq.(104) we see that in the degenerate case the rank of $\mathcal{B}$ is reduced from seven to four. From Table. 1. we se that this reduction of rank of $\mathcal{B}$ indicates a transition from entanglement class X. to class IX. The former class is the class of the state $|\Psi_-\rangle$ of Eq.(90) and the latter is the SLOCC class of the state obtained from Eq.(73) by keeping $|\omega\rangle$ with $E = F = 0$ and $D = I$ and using for $|\psi\rangle$ a state from the W-class of the Eq.(55) form.

As an other example let us consider the state

$$|\Phi_+\rangle = |\Psi_+\rangle + |\chi\rangle \tag{106}$$

where

$$|\Psi_+\rangle = (\hat{p}^{123} + \hat{p}^{1\overline{23}} + \hat{p}^{2\overline{31}} + \hat{p}^{3\overline{12}} + \hat{p}^{1\overline{14}} + \hat{p}^{2\overline{24}} + \hat{p}^{3\overline{34}})|0\rangle. \tag{107}$$

This state is labelled by the set of parameters

$$\alpha, A, B, \beta, D, E, F) = (\eta, X, Y, \xi, Z, V, U) = (1, I, 0, \xi, I, 0, U), \tag{108}$$

i.e. we have taken the negative of the matrix X. As a result of this our matrix $\mathcal{B}$ takes the following form

$$\mathcal{B}_{IJ}(\Phi_+) = \begin{pmatrix} -I & -\frac{1}{2}(\xi I - U) & -\frac{1}{2}u \\ -\frac{1}{2}(\xi I + U) & I & 0 \\ -\frac{1}{2}u^T & 0 & 1 \end{pmatrix}. \tag{109}$$

A diagonalization of $\mathcal{B}_{IJ}(\Phi_+)$ yields the eigenvalues

$$\lambda_{1,2,3} = -\sqrt{1 + \frac{1}{4}Q^2}, \qquad \lambda_{4,5,6} = \sqrt{1 + \frac{1}{4}Q^2}, \qquad \lambda_7 = 1. \tag{110}$$

Then according to Eq.(71) we have $\mathcal{J}(\Phi_+) = -\left(1 + \frac{1}{4}Q^2\right)$. Hence for ξ and U real we cannot leave the dense orbit. However, for complex parameters if the constraint $Q^2 = -4$ is satisfied then the rank of $\mathcal{B}$ is again changing from seven to four. In order to check this just take $(\xi, u^{\overline{1}}, u^{\overline{2}}, u^{\overline{3}}) = (2i, 0, 0, 0)$. In this case the matrix of Eq.(109) has a block diaginal structure containing a 6×6 block of the form $-(\sigma_3 + i\sigma_1) \otimes I$ where $\sigma_{1,3}$ are the usual Pauli matrices. However $\sigma_3 + i\sigma_1$ is of rank one, hence the 6×6 block is of rank three. Hence the matrix $\mathcal{B}(\Phi_+)$ is of rank four. Then if the constraint $Q^2 = -4$ holds the state $|\Phi_+\rangle$ will again belong to class IX.

The upshot of these considerations is as follows. Taking the perturbation parameters $\xi, u^{\overline{1}}, u^{\overline{2}}, u^{\overline{3}}$ to be real reveals an interesting effect. If we change the sign of the X parameters of the doubles (see Eqs.(91) and (108)) then the perturbation due to triples cannot induce a transition to a different SLOCC class. Hence in this special case the entanglement (which is according to Table 1. is of type X.) encoded into the parameters of the doubles is protected from the perturbating effect of the triples. On the other hand if no sign change occurs then if the perturbation parameters are constrained to lie on a three dimensional sphere of radius two, then the entanglement type is transformed to class IX. Note that the different behavior of the states $|\Psi_-\rangle$ and $|\Psi_+\rangle$ under perturbations with *real* parameters is related to the fact that these states are equivalent under complex SLOCC transformations but *inequivalent* under real ones[22].

4 The role of doubles in characterizing entanglement

Let us now address the entanglement aspects of the CC method in a somewhat more general setting. For an arbitrary number of fermions (n) and single particle states (N) one can use the coupled cluster expansion of Eq.(43). As we know from this expansion the contribution coming from singles can be removed since this merely amounts to a SLOCC transformation. Hence for the characterization of entanglement we are left with the the terms featuring the exponentials of cluster operators $\hat{T}_2, \hat{T}_3, \dots \hat{T}_n$. In this section we would like to put forward the proposal to characterize fermionic entanglement by keeping merely one of such exponentials namely the contribution coming from doubles: $\hat{T}_2$. Explicitly let us consider the approximation to $|\Psi\rangle$ of Eq.(43) in the form

$$|\Phi\rangle = e^{\hat{T}_2}|\Psi_0\rangle, \qquad \hat{T}_2 = \frac{1}{4}T_{ab}{}^{ij}\hat{p}^a\hat{n}_i\hat{p}^b\hat{n}_j \tag{111}$$

where $i, j = 1, 2, \dots n$ and $a, b = 1, 2, \dots N - n$. Naively on expects that for sufficiently small n and N the parametrization based on $\hat{T}_2$ is capable of recovering all the SLOCC classes. At the same time our parametrization of fermionic entangled states in terms of parameters of $\hat{T}_2$ is reducing the number of entanglement parameters from $\binom{N}{n}$ to $\binom{n}{2}\binom{N-n}{2}$. However, the price we have to pay is that for larger values of n and N the description of entanglement in terms of doubles can only produce a coarse graining which is generally insensitive to the fine structure of SLOCC classes. At the same time we must bear in mind that though we are losing information on the fine deatails of entanglement but at the same time this approach could be appealing from the physical point of view. Indeed, entanglement is a resource and it is the physical problem at hand that defines the criteria under which we should classify this resource. Since most of the interaction terms used in solid state, molecular and atomic physics are based on interaction terms with similar structure to that of $\hat{T}_2$ our proposal could be a valuable tool. Of course in order to check the viability of our approach investigations with realistic systems should be considered. Such investigations we would like to perform in future works. For the time being in the following we would merely like to offer some solid pieces of mathematical evidence in favour of our proposal.

Let us see first how the usual SLOCC classes are reproduced for our cases of $n = 3$, $N = 6, 7$ in terms of doubles.

In the $N = 6$ case according to Eq.(18) keeping merely the contribution from the doubles amounts to using the 3×3 matrix X for entanglement characterization. According to our discussion of SLOCC classes at the end of Section 2.3 we see that in terms of the matrix X separable states are the trivial ones with $X = X^\sharp = \mathrm{Det}X = 0$. For biseparable states we have $X \neq 0$ but $X^\sharp = \mathrm{Det}X = 0$. For the classes containing genuine entanglement the W-class has $X \neq 0$ and $X^\sharp \neq 0$ but $\mathrm{Det}X = 0$, on the other hand for the GHZ-class none of these three quantities are zero. This is in accord with Eq.(34) showing that for the GHZ class $\mathcal{D}(\Phi) = \mathrm{Det}X \neq 0$. Hence in this special case we see that a parametrization in terms of doubles intersects all of the usual SLOCC classes.

In the $N = 7$ case describing entanglement in terms of doubles means a characterization in terms of only the two 3×3 matrices

$$X^a{}_i = \frac{1}{4}\varepsilon^{abc}\varepsilon_{ijk}T_{bc}{}^{jk}, \qquad Z_{ka} = \frac{1}{2}\varepsilon_{ijk}T_{a4}{}^{ij}. \tag{112}$$

In this case $\mathcal{J}(\Phi) = -\mathrm{Det}G$ where G is the symmetric part of the matrix ZX. Hence we are in class X. of Table 1. provided this invariant is nonzero. Clearly the classes II.-V. are the ones familiar from the $N = 6$ case. In this case $Z = 0$, and the constraints are just the ones of the previous paragraph. In order to identify the constraints in terms of X and Z for the remaining classes of Table 1. one has to look at the ranks of the covariants. In particular for the calculation of the rank of the covariant N_{IJ} we have to use the expressions as displayed in the Appendix where now $\xi = 0$ and $U = 0$. Notice however, that in order to separate classes VI. and VII. further covariants are needed. For the structure of these covariants see Ref.[12].

As a less trivial example let us consider some aspects of entanglement characterization in terms of doubles for the $n = 4$, $N = 8$ case. In this case we have to use the cluster operator

$\hat{T}_2$ of Eq.(111) with $i,j=1,2,3,4$ and $a,b=\overline{1},\overline{2},\overline{3},\overline{4}$. In order to calculate $|\Phi\rangle$ of Eq.(111) we calculate

$$|\Phi\rangle = (1+\hat{T}_2+\frac{1}{2}\hat{T}_2^2)\hat{p}^{1234}|0\rangle \tag{113}$$

with

$$\hat{T}_2|\Psi_0\rangle = \frac{1}{2}({T_{ab}}^{12}\hat{p}^{34}+{T_{ab}}^{34}\hat{p}^{12}-{T_{ab}}^{13}\hat{p}^{24}-{T_{ab}}^{24}\hat{p}^{13}+{T_{ab}}^{14}\hat{p}^{23}+{T_{ab}}^{23}\hat{p}^{14})\hat{p}^{ab}|0\rangle \tag{114}$$

$$\frac{1}{2}\hat{T}_2^2|\Psi_0\rangle = \frac{1}{4}({T_{ab}}^{12}{T_{cd}}^{34}-{T_{ab}}^{13}{T_{cd}}^{24}+{T_{ab}}^{14}{T_{cd}}^{23})\varepsilon^{abcd}\hat{p}^{\overline{1234}}|0\rangle. \tag{115}$$

Since the structure of the entangelment classes in this case is quite involved[13] we are content with showing that the orbit which is closed under the SLOCC subgroup $SL(8,\mathbb{C})$ (this is a "GHZ-like" class) can be recovered by this parametrization in terms of doubles. Since almost all orbits are closed with respect to this group action[13] hence we can conclude that for all practical purposes for obtaining a coarse grained picture of entanglement this parametrization will do.(It would be interesting to check whether we are still capable of discriminating all the fine structure of SLOCC orbits, as we were in the $n=3, N=3$ case, a problem we are not addressing here.)

In order to show this the only thing we have to notice is that our parametrization with doubles obviously intersects the seven dimensional subspace spanned by the vectors obtained by acting with the following set of operators on the vacuum.

$$\hat{P}_1=\hat{p}^{1234}+\hat{p}^{\overline{1234}}, \quad \hat{P}_2=\hat{p}^{13\overline{13}}+\hat{p}^{24\overline{24}}, \quad \hat{P}_3=\hat{p}^{12\overline{12}}+\hat{p}^{34\overline{34}} \tag{116}$$

$$\hat{P}_4=\hat{p}^{13\overline{24}}+\hat{p}^{24\overline{13}}, \quad \hat{P}_5=\hat{p}^{14\overline{14}}+\hat{p}^{23\overline{23}}, \quad \hat{P}_6=-\hat{p}^{14\overline{23}}-\hat{p}^{23\overline{14}}, \quad \hat{P}_7=-\hat{p}^{12\overline{34}}-\hat{p}^{34\overline{12}}. \tag{117}$$

According to Ref.[13] the closed orbits are precisely those that meet this subspace generated by the vectors above. Indeed, choosing

$${T_{\overline{12}}}^{12}={T_{\overline{34}}}^{34}=a, \quad {T_{\overline{12}}}^{34}={T_{\overline{34}}}^{12}=b, \quad {T_{\overline{13}}}^{13}={T_{\overline{24}}}^{24}=c, \quad {T_{\overline{24}}}^{13}={T_{\overline{13}}}^{24}=d, \tag{118}$$

$${T_{\overline{14}}}^{14}={T_{\overline{23}}}^{23}=e, \quad {T_{\overline{23}}}^{14}={T_{\overline{14}}}^{23}=f, \quad a^2+b^2-c^2-d^2+e^2+f^2=1 \tag{119}$$

shows that $|\Phi\rangle$ will be a state in the subspace spanned by $\hat{P}_I|0\rangle, I=1,2,\dots 7$.

5 Conclusions

In this paper by studying simple fermionic systems we established a connection between the Coupled Cluster (CC) Method and quantum entanglement. In the CC method for n-fermions with N modes one starts with a single Slater determinant comprising a special set of n single particle states, called the *occupied ones*. Then to this distinguished state one applies a commuting set of cluster operators of the form $e^{\hat{T}_i}, i=1,2,\dots n$. We have initiated a study of the problem how these cluster operators are encoding the SLOCC entanglement properties of the system via complex expansion coefficients of operator combinations called singles, doubles, triples etc. These operators are describing transitions from the occupied modes to the non-occupied ones. Our starting point was the simple observation that the operator $e^{\hat{T}_1}$ featuring singles is a special fermionic SLOCC transformation. Indeed, the transformation $|\Psi\rangle \mapsto e^{\hat{T}_1}|\Psi\rangle$ can be rewritten in the form $|\Psi\rangle \mapsto S\otimes S\otimes\cdots\otimes S|\Psi\rangle$ meaning

$$\Psi_{\mu_1\mu_2\dots\mu_n} \mapsto {S_{\mu_1}}^{\nu_1}{S_{\mu_2}}^{\nu_2}\cdots {S_{\mu_n}}^{\nu_n}\Psi_{\nu_1\nu_2\dots\nu_n}, \qquad S\in GL(N,\mathbb{C}) \tag{120}$$

with S an $N\times N$ matrix having the (36) structure. As a result of this in order to study SLOCC entanglement we merely have to look at the structure of the cluster operators $\hat{T}_2, \hat{T}_3, \dots \hat{T}_n$.

In order to make some progress in clarifying how multipartite entanglement manifests itself in these operators we conducted a study on the simplest nontrivial cases of $n = 3$ and $N = 6, 7$. In these cases the structure of the SLOCC classes and the structure of the invariants and covariants is explicitely known. Surprisingly in the special case of six modes the CC expansion is tailor made to characterize the usual SLOCC entanglement classes. It means that the notion of a SLOCC transformation shows up quite naturally as a one relating the CC and CI expansions , and going from the CI expansion to the CC one is equivalent to obtaining a canonical form for the state where the structure of the entanglement classes is transparent. Using the CC parametrization of states (Eqs.(16)-(18) and Eqs.(75)-(80)) in the six and seven mode cases we have given simple expressions for the unique SLOCC invariants $\mathcal{D}$ and $\mathcal{J}$ (see Eqs.(34) and (81)) serving as natural measures of multipartite entanglement[9, 11, 12]. In the six mode case we have given a full characteriation of the SLOCC entanglment classes in terms of the cluster operators corresponding to doubles and triples. In the seven mode case we have considered a perturbation problem featuring a state from the unique SLOCC class characterized by $\mathcal{J} \neq 0$. For this state with entanglement generated by doubles we investigated the phenomenon of changing the entanglement type due to the perturbing effect of triples. For the representative of the dense orbit (class X.) we have chosen a "GHZ-like" state generated by doubles. We then used the four complex parameters characterizing the triples as perturbations. We have shown that when these parameters define a deformed conifold with a deformation parameter $Q = 2$ then a transition to a new entanglement class (class IX.) is possible. We have also demonstrated that there are states with real amplitudes such that their entanglement encoded into configurations of clusters of doubles is protected from errors generated by triples.

The results of this paper were primary aimed at drawing the readers attention to the existence of the connection between multipartite fermionic entanglement and the structure of coupled cluster operators. A natural question to be asked is how our results illustrated merely in the simplest nontrivial multipartite (i.e. tripartite) cases generalize to more realistic ones which are containing genuine multipartite systems with an arbitrary number of modes. A promising idea in this respect seems to consider entanglement characterization via doubles meaning by the entanglement parameters showing up in the cluster operator $\hat{T}_2$. Dealing with merely doubles is reducing the entanglement parameters that we have to account for, but at the same time we are loosing some of the finer details provided by the usual SLOCC classification. However, entanglement is a resource and it is the physical problem at hand that defines the criteria under which we should classify this resource. Since interactions based on exchange processes involving pairs of modes (particles) are common in physics, an appreciation of this idea could provide a basis for further elaborations of our proposal.

In order to fully explore the connection found here between entnaglement and the CC-method there are many possible avenues to follow. Obviously the most important of such vistas would be a demonstration how the entanglement encoded in the cluster operators can be used for studying the properties of realistic (e.g. three electron) systems. Such ideas we are intending to explore in future work. Another mainly theoretical line of development would be to invoke further results from the theory of spinors[27, 28, 29, 30]. In particular in order to investigate entanglement patterns one has to use the natural invariants defined for spinors[28, 29, 30, 31, 14], and possibly other notions such as the nullity of a spinor[30]. Hopefully these structures will provide a further insight into the coarse grained structure of entanglement types based on the CC method.

6 Appendix

Here for the convenience of the reader for the seven single particle case we give the explicit form of the covariants N_{IJ} and L^{IJ} in terms of the relevant coupled cluster parameters (ξ, X, Z, U). In the expressions below X and Z and U are complex 3×3 matrices where U is antisymmetric hence it can also be parametrized as $U_{ab} = \varepsilon_{abc} u^c$ with u^c a three component vector. Recall the index structures Z_{ia}, ${X^a}_i$, $(Z^\sharp)^{ai}$ and ${(X^\sharp)^i}_a$ which are being in accord

with expressions like $Z_{ia}(Z^\sharp)^{aj} = (\mathrm{DetZ})\delta_i{}^j$ etc.

$$N_{ij} = 3[ZX + (ZX)^T]_{ij}, \qquad N_{ab} = -3[Z^T X^\sharp + (Z^T X^\sharp)^T]_{ab}, \qquad N_{77} = -6\mathrm{Det}Z \quad (121)$$

$$N_{ai} = 3(UX + \xi Z^T)_{ai}, \qquad N_{i7} = 3(Zu)_i, \qquad N_{a7} = -3\varepsilon_{abc}(XZ^{T\sharp})^{bc}. \quad (122)$$

$$L^{ij} = -6[(ZX)^\sharp + (ZX)^{T\sharp}] - 3\varepsilon^{ikl}\varepsilon^{jmn}[(ZX)_{km}(ZX)^T_{ln} + (ZX)^T_{km}(ZX)_{ln}] \quad (123)$$

$$L^{ab} = 12[(XZ^{T\sharp}) + (XZ^{T\sharp})^T]^{ab} + 6u^a u^b, \qquad L^{77} = 6[\xi^2 + 4\mathrm{Det}X]. \quad (124)$$

$$L^{ai} = 12\varepsilon^{ijk}X^a{}_j(Zu)_k + 6\varepsilon^{ijk}u^a(ZX)_{jk} - 12\xi(Z^\sharp)^{ai} \quad (125)$$

$$L^{i7} = 6\xi\varepsilon^{ijk}(ZX)_{jk} - 6\varepsilon^{ijk}U_{ab}X^a{}_j X^b{}_k, \qquad L^{a7} = -6\xi u^a + 12\varepsilon^{abc}(Z^T X^\sharp)_{bc}. \quad (126)$$

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